Access DB# 87910

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKEY Examiner #: 73489 Date: 3/3/03
Art Unit: 1626 Phone Number 305-6889 Serial Number: 10/662,579
Mail Box and Bldg/Room Location: CM1 3B19 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. MEJ

****

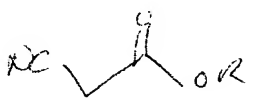
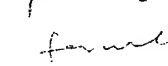
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Method for producing Cyanoacetic acid Esters

Inventors (please provide full names): Paul Hanselmann et al

Earliest Priority Filing Date: 8/30/99

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

A process for preparing Cyanoacetic acid ester of formula  comprising oxidizing alkoxypropionitrile of formula  wherein R is optionally substituted alkyl or branched C_{1-8} alkyl or an aryl & C_{1-4} alkyl group containing oxygen or oxygen bearing reagent in the presence of a catalyst based on lead or one of the transition metals.

Jan Delavai
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

****

STAFF USE ONLY

Searcher: [illegible]
Searcher Phone #: 4478
Searcher Location: _____
Date Searcher Picked Up: 3/10/03
Date Completed: 3/10/03
Searcher Prep & Review Time: _____
Clerical Prep Time: 10
Online Time: 1.25

Type of Search

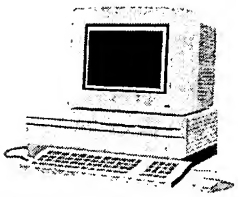
NA Sequence (#) _____
AA Sequence (#) _____
Structure (#) L
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other _____

Vendors and cost where applicable

STN C
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
Sequence Systems _____
WWW/Internet _____
Other (specify) _____

PTO-1590 (8-01)

BioTech-Chem Library
Search Results
Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact ***the BioTech-Chem searcher*** who conducted the search ***or contact***:

Mary Hale, Supervisor, 308-4258
CM-1 Room 1E01

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* *(Example: 1610)*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

  Types of relevant prior art found:
  - ☐ Foreign Patent(s)
  - ☐ Non-Patent Literature
    (journal articles, conference proceedings, new product announcements etc.)
- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Search results were not useful in determining patentability or understanding the invention.

Other Comments:

Drop off completed forms at the **Circulation Desk CM-1,** or send to Mary Hale, **CM1-1E01 or e-mail mary.hale@uspto.gov.**

=> fil casreact
FILE 'CASREACT' ENTERED AT 07:43:47 ON 10 MAR 2003

FILE CONTENT:1907 - 9 Mar 2003 VOL 138 ISS 10

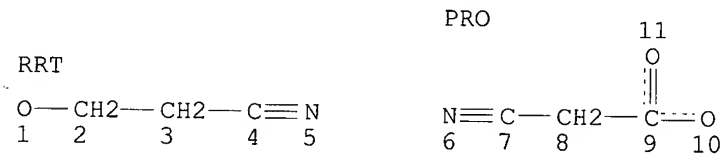
Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> d sta que l5
L3 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L5 2 SEA FILE=CASREACT SSS FUL L3 (4 REACTIONS)

100.0% DONE 10260 VERIFIED 4 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.01

=> d l5 bib abs fhit retable tot

L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 134:207549 CASREACT
TI Oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles
IN Hanselmann, Paul; Hildbrand, Stefan
PA Lonza A.-G., Switz.
SO PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DT Patent
LA German

FAN.CNT 1

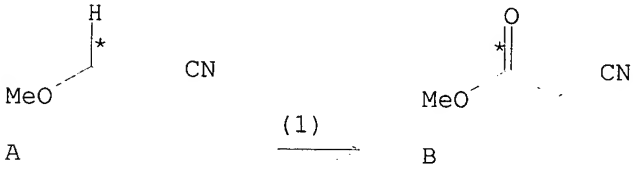
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 20Q1016092	A1	20010308	WO 2000-EP8397	20000829
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208081	A1	20020529	EP 2000-964050	20000829
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRAI EP 1999-117033 19990830
US 2000-185372P 20000228
WO 2000-EP8397 20000829

OS MARPAT 134:207549

AB Cyanoacetate esters NCCH2CO2R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepd. in high yield and selectivity by the oxidn. of 3-(alkoxy)propionitriles RO(CH2)2CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).

RX(1) OF 3 **A** ===> **B**



RX(1) RCT A **110-67-8**

STAGE(1)
RGT C 524-38-9 N-Hydroxyphthalimide
CAT 6147-53-1 Acetic acid, cobalt(2+) salt, tetrahydrate
SOL 64-19-7 AcOH

STAGE(2)
RGT D 7782-44-7 O2
PRO B **105-34-0**

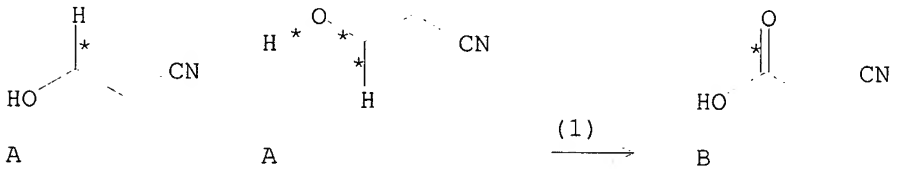
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Catalytcca Inc	1992			WO 9212962 A	CAPLUS
Matsui, K	1984			US 4438041 A	CAPLUS
Wermeckes, B	1985	118	3771	CHEM BER	CAPLUS
Wermeckes, B	1985	30	1491	ELECTROCHIM ACTA	CAPLUS

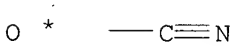
L5 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 103:214838 CASREACT
TI Anodic oxidation of 2-cyanoethanol to cyanoacetic acid
AU Wermeckes, Bernd; Beck, Fritz

CS GH, Univ. Duisburg, Duisburg, D-4100/1, Fed. Rep. Ger.
SO Chemische Berichte (1985), 118(9), 3771-80
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
AB 2-Cyanoethanol was oxidized electrochem. to cyanoacetic acid in aq. H2SO4 at Pt and PbO2 anodes (current densities of 30-200 mA cm-2). Current efficiencies and material yields were up to 60%. Side products were HCN (via an anodic attack at .beta.-CH2) and cyanoacetaldehyde, with 8-15 and 3-13% current efficiencies on Pt. In principle, HCN can be recycled to new starting material and cyanoacetaldehyde to yield further product. Electrooxidn. at Pt takes place at an anode which is partially covered with platinum oxides. High over-voltages are interpreted in terms of a voltage drop in a rigid org. adsorbate layer.

RX(1) OF 1 2 **A** ===> **B** + C



A A B



C

RX(1) RCT A **109-78-4**
RGT D 7664-93-9 H2SO4
PRO B **372-09-8**, C 6162-76-1
SOL 7732-18-5 Water
NTE Anodic oxidn.

=> fil reg
FILE 'REGISTRY' ENTERED AT 08:01:32 ON 10 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2003 HIGHEST RN 497220-90-3
DICTIONARY FILE UPDATES: 9 MAR 2003 HIGHEST RN 497220-90-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

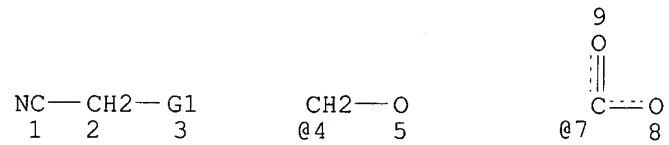
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties

in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

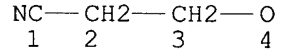
=> d sta que l11
L6 STR



VAR G1=4/7
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L8 14129 SEA FILE=REGISTRY SSS FUL L6
L9 STR



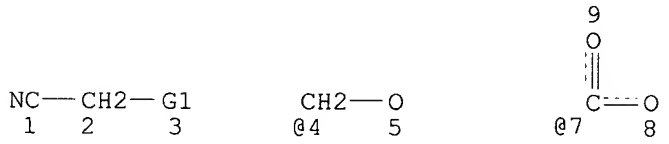
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE
L11 13071 SEA FILE=REGISTRY SUB=L8 SSS FUL L9

100.0% PROCESSED 13996 ITERATIONS 13071 ANSWERS
SEARCH TIME: 00.00.01

=> d sta que l13
L6 STR

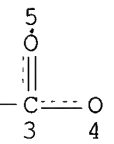


VAR G1=4/7
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

```
L8         14129 SEA FILE=REGISTRY SSS FUL L6
L12               STR
```




```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L13         1059 SEA FILE=REGISTRY SUB=L8 SSS FUL L12

100.0% PROCESSED   4883 ITERATIONS                      1059 ANSWERS
SEARCH TIME: 00.00.01


=> d his

     (FILE 'HOME' ENTERED AT 07:40:07 ON 10 MAR 2003)
               SET COST OFF

     FILE 'CASREACT' ENTERED AT 07:40:32 ON 10 MAR 2003
L1             STR
L2           0 S L1
L3             STR L1
L4           0 S L3
L5           2 S L3 FUL
               SAV L5 SACKEY069/A

     FILE 'CASREACT' ENTERED AT 07:43:47 ON 10 MAR 2003

     FILE 'REGISTRY' ENTERED AT 07:44:12 ON 10 MAR 2003
L6             STR
L7            50 S L6
L8         14129 S L6 FUL
               SAV TEMP L8 SACKEY069A/A
L9             STR
L10           50 S L9 SAM SUB=L8
L11        13071 S L9 FUL SUB=L8
               SAV TEMP L11 SACKEY069B/A
L12            STR L9
L13         1059 S L12 FUL SUB=L8
               SAV L13 SACKEY069C/A
               E COBALT/CN
L14            1 S E3
L15            9 S COBALT (L) ACETATE (L) TETRAHYDRATE
L16            1 S L15 AND C2H4O2 AND H2O AND 3/NC
L17           17 S 64-19-7/CRN AND CO/ELS AND H2O
L18           14 S L17 AND 3/NC
L19           10 S L18 NOT N/ELS
               E LEAD/CN
L20            1 S E3
               E T/HP
               E TR/HP
```

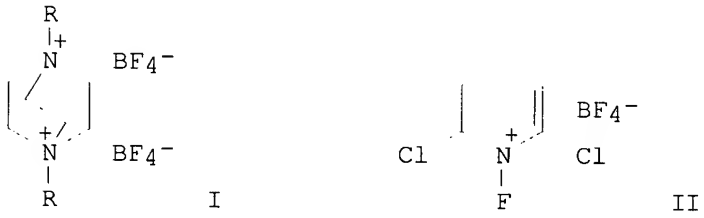
```
                E T/PG
                E A/PG
L21          6423 S E23-E25 AND 1/ELC.SUB
L22          3889 S L21 NOT ISOTOPE
L23          1340 S L22 AND 1/ATC
L24            38 S L23 NOT ION

     FILE 'HCAPLUS' ENTERED AT 07:52:34 ON 10 MAR 2003
L25          7333 S L13
L26          8502 S L11
L27            79 S L25 AND L26
L28             2 S L27 AND L14,L16,L19,L20,L24
L29            13 S L13/P AND L27
L30          4517 S L26 (L) (RCT OR RACT OR RGT)/RL
L31            41 S L30 AND L27
L32             5 S L29 AND L31
L33             5 S L28,L32

     FILE 'REGISTRY' ENTERED AT 07:55:12 ON 10 MAR 2003
L34             1 S OXYGEN/CN

     FILE 'HCAPLUS' ENTERED AT 07:55:17 ON 10 MAR 2003
L35             1 S L27 AND L34
L36             5 S L33,L35
                E HANSELMANN P/AU
L37            17 S E4
                E HILDBRAND S/AU
L38            14 S E4
                E LONZA/PA,CS
L39          1853 S E3,E4
L40             1 S L37,L38,L39 AND L27
L41             6 S L37,L38,L39 AND L26
L42             5 S L36,L40
L43             5 S L41 NOT L42

     FILE 'USPATFULL, USPAT2' ENTERED AT 07:56:53 ON 10 MAR 2003
L44          1971 S L11
L45          1636 S L13
L46            25 S L44 AND L45
L47             0 S L46 AND L14,L16,L19,L20,L24,L34
L48            21 S L46 AND (PB OR LEAD OR CO OR COBALT OR TRANSITION METAL OR OX
L49             6 S L11/P AND L46
L50             6 S L48 AND L49
L51             0 S L49 AND COBALT

     FILE 'IFIPAT' ENTERED AT 08:00:48 ON 10 MAR 2003

     FILE 'REGISTRY' ENTERED AT 08:01:32 ON 10 MAR 2003

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:01:45 ON 10 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE COVERS 1907 - 10 Mar 2003 VOL 138 ISS 11
FILE LAST UPDATED: 9 Mar 2003 (20030309/ED)

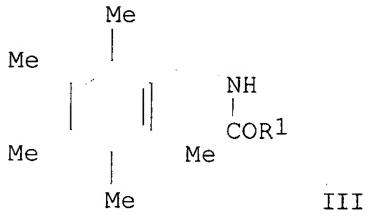
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 142

L42 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:508660 HCAPLUS
DN 135:272730
TI Effective and versatile functionalisation of hexamethylbenzene using N-F reagents
AU Stavber, Stojan; Kralj, Petra; Zupan, Marko
CS Laboratory for Organic and Bioorganic Chemistry, "Jozef Stefan" Institute and Department of Chemistry, University of Ljubljana, Ljubljana, 1000, Slovenia
SO Synlett (2001), (7), 1152-1154
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 135:272730
GI



I II



III

AB Effective direct introduction of alkoxy, amino, azido or halogeno functional groups on the benzylic position in hexamethylbenzene was mediated by the electrophilic fluorinating (N-F) reagents I (R = ClCH2, HO), (PhSO2)2NF and II in the presence of alcs., carboxylic acids, cyanides or trimethylsilyl derivs. as sources of an external nucleophile. Thus, aryl amides III [R1 = Et, Me(CH2)4, Me2CH, cyclopropyl, MeOCH2, MeO2CCH2, EtO2CCH2, Ph, 4-MeO2CC6H4, PhCH2] were prepd. from the reaction of hexamethylbenzene and R1CONH2 mediated by I (R = ClCH2) in 65-98% yield.

ST ether benzyl prepn; nucleophile methylbenzene substitution electrophilic

fluorinating reagent mediated; etherification alc methylbenzene electrophilic fluorinating reagent mediated; amidation nitrile methylbenzene electrophilic fluorinating reagent mediated; amide benzyl prepn; benzylic functionalisation methylbenzene electrophilic fluorinating reagent

IT Fluorination
(agents, electrophilic; prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

IT Amides, preparation
Ethers, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(benzyl; prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

IT Amidation
(prepn. of pentamethylphenylmethyl amides via electrophilic fluorinating reagent-mediated amidation of hexamethylbenzene with nitriles)

IT Nucleophiles
(prepn. of pentamethylphenylmethyl derivs. via electrophilic fluorinating reagent-mediated substitution of hexamethylbenzene with nucleophiles)

IT Alcohols, reactions
Nitriles, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

IT Substitution reaction
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with alcs. and nitriles)

IT Etherification
(prepn. of pentamethylphenylmethyl ethers via electrophilic fluorinating reagent-mediated etherification of hexamethylbenzene with alcs.)

IT **109-78-4**, 2-Cyanoethanol
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)

IT **363148-38-3P** 363148-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)

IT **7062-95-5**, Potassium cyanoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)

IT **363148-37-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)

IT **372-09-8**, 2-Cyanoacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoacetic acid in TFA)

IT 363148-36-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoacetic acid in TFA)

IT 484-65-1P 243118-23-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl azide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with TMS azide)

IT 19936-85-7P 35843-80-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl esters via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with carboxylic acids)

IT 67-63-0, 2-Propanol, reactions 75-89-8, 2,2,2-Trifluoroethanol 78-82-0, 2-Cyanopropane 87-85-4, Hexamethylbenzene 96-41-3, Cyclopentanol 100-47-0, Benzonitrile, reactions 100-51-6, Benzyl alcohol, reactions **105-34-0**, Methyl 2-cyanoacetate **105-56-6**, Ethyl 2-cyanoacetate 107-12-0, Propionitrile 109-86-4, 2-Methoxyethanol 111-27-3, 1-Hexanol, reactions 140-29-4, Benzylnitrile 628-73-9, Hexanenitrile 1129-35-7, Methyl 4-cyanobenzoate 1738-36-9, Methoxyacetonitrile 5500-21-0, Cyclopropanenitrile 133745-75-2, N-Fluorobenzenesulfonimide 140623-89-8, N-Fluoro-2,6-dichloropyridinium tetrafluoroborate 140681-55-6, Selectfluor 172090-26-5, 1-Fluoro-4-hydroxy-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate)
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

IT 64512-95-4P 363148-21-4P 363148-22-5P 363148-23-6P 363148-24-7P 363148-25-8P 363148-26-9P 363148-27-0P 363148-28-1P 363148-29-2P 363148-30-5P 363148-31-6P 363148-32-7P 363148-33-8P 363148-34-9P 363148-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

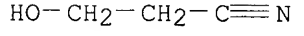
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

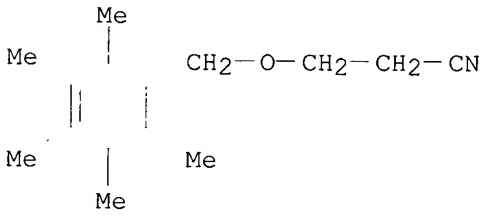
(1) Anon; Methods of Organic Chemistry (Houben-Weyl) 1999, VE 10a and 10b
(2) Bewick, A; Liebigs Ann Chem 1978, P41 HCAPLUS
(3) Bishop, R; Comprehensive Organic Synthesis 1991, V6 HCAPLUS
(4) Dalla Cort, A; J Chem Res S 1983, P44 HCAPLUS
(5) Dalla Cort, A; Synth Commun 1988, V18, P613 HCAPLUS
(6) Differding, E; Tetrahedron 1992, V48, P1595 HCAPLUS
(7) Eberson, L; Acta Chem Scan B 1978, V32, P157
(8) Furin, G; Russian Chem Rev 1999, V68, P653 HCAPLUS
(9) Gilicinski, A; J Fluorine Chem 1992, V59, P157 HCAPLUS
(10) Lal, G; Chem Rev 1996, V96, P1737 HCAPLUS
(11) Lal, G; J Org Chem 1993, V58, P2791 HCAPLUS
(12) Lau, W; J Org Chem 1984, V106, P6720
(13) Maini, S; J Org Chem 1978, V43, P3236 HCAPLUS
(14) Singh, S; J Am Chem Soc 1987, V109, P7194 HCAPLUS
(15) Sket, B; J Org Chem 1978, V43, P835 HCAPLUS
(16) Stavber, S; J Org Chem 1983, V48, P2223 HCAPLUS
(17) Stavber, S; J Org Chem 1991, V56, P7347 HCAPLUS
(18) Suzuki, H; Bull Chem Soc 1968, V41, P2197 HCAPLUS
(19) Taylor, S; Tetrahedron 1999, V55, P12431 HCAPLUS
(20) Visser, G; J Org Chem 1986, V51, P1886 HCAPLUS
(21) Wasserman, H; J Org Chem 1971, V36, P1765 HCAPLUS
(22) Zupan, M; Chimia 1976, V30, P305 HCAPLUS

IT **109-78-4**, 2-Cyanoethanol

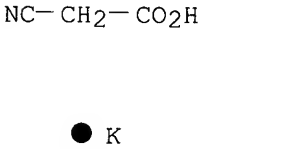
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)
RN 109-78-4 HCAPLUS
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



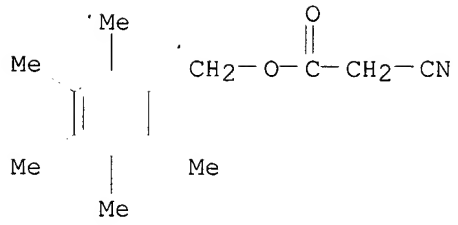
IT **363148-38-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)
RN 363148-38-3 HCAPLUS
CN Propanenitrile, 3-[(pentamethylphenyl)methoxy]- (9CI) (CA INDEX NAME)



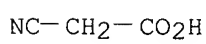
IT **7062-95-5**, Potassium cyanoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)
RN 7062-95-5 HCAPLUS
CN Acetic acid, cyano-, potassium salt (8CI, 9CI) (CA INDEX NAME)



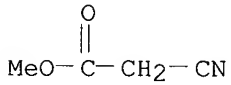
IT **363148-37-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)
RN 363148-37-2 HCAPLUS
CN Acetic acid, cyano-, (pentamethylphenyl)methyl ester (9CI) (CA INDEX NAME)



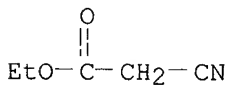
IT **372-09-8**, 2-Cyanoacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoacetic acid in TFA)
RN 372-09-8 HCAPLUS
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **105-34-0**, Methyl 2-cyanoacetate **105-56-6**, Ethyl 2-cyanoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)
RN 105-34-0 HCAPLUS
CN Acetic acid, cyano-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 105-56-6 HCAPLUS
CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



L42 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:167957 HCAPLUS
DN 134:207549
TI Oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles
IN **Hanselmann, Paul; Hildbrand, Stefan**
PA **Lonza** A.-G., Switz.
SO PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07C253-30
ICS C07C255-19
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 45, 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016092	A1	20010308	WO 2000-EP8397	20000829
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208081	A1	20020529	EP 2000-964050	20000829
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	EP 1999-117033	A	19990830		
	US 2000-185372P	P	20000228		
	WO 2000-EP8397	W	20000829		

OS CASREACT 134:207549; MARPAT 134:207549

AB Cyanoacetate esters NCCH2CO2R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepd. in high yield and selectivity by the oxidn. of 3-(alkoxy)propionitriles RO(CH2)2CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).

ST cyanoacetate ester prepn oxidn alkoxypropionitrile; catalyst oxidn alkoxypropionitrile prepn cyanoacetate ester; methyl cyanoacetate prepn methoxypropionitrile oxidn

IT Organic compounds, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyano, 3-(alkoxy)propionitriles; oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)

IT Oxidation
(liq.-phase, .0; of 3-(alkoxy)propionitriles into cyanoacetate esters)

IT Oxidation catalysts
(liq.-phase; lead or transition metals for the conversion of 3-(alkoxy)propionitriles into cyanoacetate esters)

IT Transition metals, uses
RL: CAT (Catalyst use); USES (Uses)
(oxidn. catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)

IT **110-67-8**, 3-Methoxypropionitrile 524-38-9, N-Hydroxyphthalimide **2141-62-0**, 3-Ethoxypropionitrile **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)

IT **105-34-0P**, Methyl 2-cyanoacetate **105-56-6P**, Ethyl 2-cyanoacetate
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)

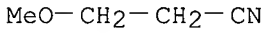
IT **6147-53-1**, Cobalt diacetate tetrahydrate **7439-92-1**, Lead, uses
RL: CAT (Catalyst use); USES (Uses)
(oxidn. catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

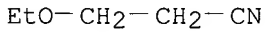
RE

(1) Catalytcca Inc; WO 9212962 A 1992 HCAPLUS
(2) Matsui, K; US 4438041 A 1984 HCAPLUS
(3) Wermeckes, B; CHEM BER 1985, V118(9), P3771 HCAPLUS

(4) Wermeckes, B; ELECTROCHIM ACTA 1985, V30(11), P1491 HCAPLUS
IT **110-67-8**, 3-Methoxypropionitrile **2141-62-0**, 3-Ethoxypropionitrile **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)
RN 110-67-8 HCAPLUS
CN Propanenitrile, 3-methoxy- (9CI) (CA INDEX NAME)

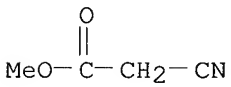


RN 2141-62-0 HCAPLUS
CN Propanenitrile, 3-ethoxy- (9CI) (CA INDEX NAME)

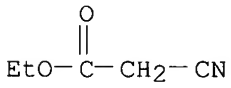


RN 7782-44-7 HCAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

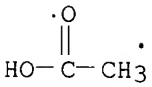
IT **105-34-0P**, Methyl 2-cyanoacetate **105-56-6P**, Ethyl 2-cyanoacetate
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)
RN 105-34-0 HCAPLUS
CN Acetic acid, cyano-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 105-56-6 HCAPLUS
CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **6147-53-1**, Cobalt diacetate tetrahydrate **7439-92-1**, Lead, uses
RL: CAT (Catalyst use); USES (Uses)
(oxidn. catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)
RN 6147-53-1 HCAPLUS
CN Acetic acid, cobalt(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

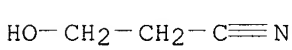
●2 H_2O

RN 7439-92-1 HCAPLUS
CN Lead (8CI, 9CI) (CA INDEX NAME)

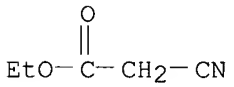
Pb

L42 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS
AN 1988:94057 HCAPLUS
DN 108:94057
TI Convenient synthesis for selectively isotopically labeled acrylonitriles
AU Van den Berg, E. M. M.; Richardson, E. E.; Lugtenburg, J.; Jenneskens, L. W.
CS Gorlaeus Lab., Univ. Leiden, Leiden, 2300 RA, Neth.
SO Synthetic Communications (1987), 17(10), 1189-98
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
CC 23-19 (Aliphatic Compounds)
OS CASREACT 108:94057
AB Short syntheses of CH2:CHCN (I) and HOCH2CH2CN (II) which can be used to prep. isotopically labeled I are reported. Thus, HOCH2CH2Br reacted with KCN to give II, which was treated with Ac2O to give AcOCH2CH2CN. Flash vacuum thermolysis of the latter compd. gave I in near quant. yield.
ST labeled acrylonitrile prepn; cyanoethyl acetate prepn elimination
IT Elimination reaction
(of cyanoethyl acetate, acrylonitrile from)
IT 105-58-8, Diethyl carbonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of lithiated acetonitrile)
IT 75-05-8, Acetonitrile, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and acylation of, with di-Et carbonate)
IT **109-78-4P**, 2-Cyanoethanol
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(prepn. and acetylation of)
IT **105-56-6P**, Ethyl .alpha.-cyanoacetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and borohydride redn. of)
IT **5325-93-9P**, 2-Cyanoethyl acetate
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and elimination of acetic acid from)
IT **372-09-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

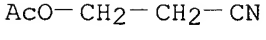
(prepn. and esterification of)
IT 107-13-1P, Acrylonitrile, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as model synthesis of labeled derivs. of)
IT 79-08-3, .alpha.-Bromoacetic acid 540-51-2, 2-Bromoethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with cyanide)
IT **109-78-4P**, 2-Cyanoethanol
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(prepn. and acetylation of)
RN 109-78-4 HCAPLUS
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



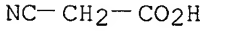
IT **105-56-6P**, Ethyl .alpha.-cyanoacetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and borohydride redn. of)
RN 105-56-6 HCAPLUS
CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **5325-93-9P**, 2-Cyanoethyl acetate
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and elimination of acetic acid from)
RN 5325-93-9 HCAPLUS
CN Propanenitrile, 3-(acetyloxy)- (9CI) (CA INDEX NAME)



IT **372-09-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)
RN 372-09-8 HCAPLUS
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



L42 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS
AN 1986:41890 HCAPLUS
DN 104:41890
TI Anodic oxidation of .beta.-cyanoethyl ethers
AU Wermeckes, B.; Beck, F.
CS Univ. Duisburg, Duisburg, D 4100/1, Fed. Rep. Ger.
SO Electrochimica Acta (1985), 30(11), 1491-500
CODEN: ELCAAV; ISSN: 0013-4686
DT Journal
LA English

CC 72-4 (Electrochemistry)
Section cross-reference(s): 23

AB Anodic oxidn. of .beta.-cyanoethyl ethers ROCH2CH2CN (R = Me, Et, tert-Bu, CH2CH2CN) was carried out in 1.6M H2SO4, using Pt and PbO2 as anodes. The main products were cyanoacetic acid (CEA) and the acid corresponding to R (HCOOH for R = Me, HOAc for R = Et). In the case of R = Et (EPN), HOAc was found with current efficiencies up to 81% (at low conversions), while CEA was generated with relatively low current efficiencies .ltoreq.34%. Kinetic curves for EPN exhibit an early appearance of .beta.-oxypropionitrile (OPN), the intermediate to CEA, and acetaldehyde. Thus, the -CH2 group of Et is primarily attacked to yield the semiacetal in a 2 electron oxidn., which is rapidly cleaved in acid solns. to yield the above-mentioned intermediates. HCN found as a side product is derived from anodic attack at the -CH2 group adjacent to the cyano group, leading to the readily sapond. cyanohydrin. The ether reacts in the adsorbed state. This leads to large pos. potential shifts and unusual Tafel slopes of 240-300 mV decade-1 due to only partial efficiency of Galvani voltage. Moreover, a partial coverage of Pt electrode with PtOx was detected even in the presence of the ether. Coincidence of PtOx-potential and initial oxidn. potential of ether leads to the proposal of a mechanism in terms of redox catalysis. Et2O is oxidized to HOAc in high yields. Thus, these findings are not restricted to .beta.-cyanoethyl ethers.

ST cyanoethyl ether electrooxidn; methyl cyanoethyl ether electrooxidn; ethyl cyanoethyl ether electrooxidn; butyl cyanoethyl ether electrooxidn; alkyl cyanoethyl ether electrooxidn; lead oxide anode cyanoethyl ether; platinum anode cyanoethyl ether oxidn; cyanoacetic acid electroprepn cyanoethyl ether; formic acid electroprepn cyanoethyl ether; acetic acid electroprepn cyanoethyl ether

IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanoethyl, oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)

IT Electric current
(efficiency of, in oxidn. of .beta.-cyanoethyl ethers on lead oxide or platinum in sulfuric acid)

IT Oxidation, electrochemical
(of .beta.-cyanoethyl ethers, on lead oxide or platinum in sulfuric acid)

IT Electric potential
(oxidn., of cyano compds. in sulfuric acid)

IT **7440-06-4**, uses and miscellaneous
RL: USES (Uses)
(anodes, for oxidn. of .beta.-cyanoethyl ethers)

IT 1309-60-0
RL: PRP (Properties)
(anodes, for oxidn. of .beta.-cyanoethyl ethers)

IT 7664-93-9, uses and miscellaneous
RL: USES (Uses)
(electrochem. oxidn. of .beta.-cyanoethyl ethers on lead dioxide or platinum in soln. contg.)

IT 50-00-0P, preparation 74-90-8P, preparation 75-07-0P, preparation **109-78-4P** 6162-76-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidn. of .beta.-cyanoethyl ethers)

IT 60-29-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of, electrochem., on lead oxide or platinum)

IT **110-67-8 1656-48-0 2141-62-0** 33573-94-3 **99764-73-5**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)

IT 11129-89-8
RL: PRP (Properties)

(platinum electrode contg., oxidn. of .beta.-cyanoethyl ethers on)
IT 64-18-6P, preparation 64-19-7P, preparation **372-09-8P**
RL: PREP (Preparation)
(prepn. of, by electrochem. oxidn. of .beta.-cyanoethyl ethers)
IT **7440-06-4**, uses and miscellaneous
RL: USES (Uses)
(anodes, for oxidn. of .beta.-cyanoethyl ethers)
RN 7440-06-4 HCAPLUS
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT **109-78-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidn. of .beta.-cyanoethyl ethers)
RN 109-78-4 HCAPLUS
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)

HO—CH_2—CH_2—C≡N

IT **110-67-8 1656-48-0 2141-62-0**
99764-73-5
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)
RN 110-67-8 HCAPLUS
CN Propanenitrile, 3-methoxy- (9CI) (CA INDEX NAME)

MeO—CH_2—CH_2—CN

RN 1656-48-0 HCAPLUS
CN Propanenitrile, 3,3'-oxybis- (9CI) (CA INDEX NAME)

NC—CH_2—CH_2—O—CH_2—CH_2—CN

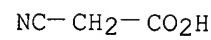
RN 2141-62-0 HCAPLUS
CN Propanenitrile, 3-ethoxy- (9CI) (CA INDEX NAME)

EtO—CH_2—CH_2—CN

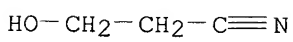
RN 99764-73-5 HCAPLUS
CN Propanenitrile, 3-(1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)

t-BuO—CH_2—CH_2—CN

IT **372-09-8P**
RL: PREP (Preparation)
(prepn. of, by electrochem. oxidn. of .beta.-cyanoethyl ethers)
RN 372-09-8 HCAPLUS
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



L42 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
AN 1985:614838 HCAPLUS
DN 103:214838
TI Anodic oxidation of 2-cyanoethanol to cyanoacetic acid
AU Wermeckes, Bernd; Beck, Fritz
CS GH, Univ. Duisburg, Duisburg, D-4100/1, Fed. Rep. Ger.
SO Chemische Berichte (1985), 118(9), 3771-80
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
CC 23-16 (Aliphatic Compounds)
Section cross-reference(s): 72
OS CASREACT 103:214838
AB 2-Cyanoethanol was oxidized electrochem. to cyanoacetic acid in aq. H2SO4 at Pt and PbO2 anodes (current densities of 30-200 mA cm-2). Current efficiencies and material yields were up to 60%. Side products were HCN (via an anodic attack at .beta.-CH2) and cyanoacetaldehyde, with 8-15 and 3-13% current efficiencies on Pt. In principle, HCN can be recycled to new starting material and cyanoacetaldehyde to yield further product. Electrooxidn. at Pt takes place at an anode which is partially covered with platinum oxides. High over-voltages are interpreted in terms of a voltage drop in a rigid org. adsorbate layer.
ST hydroxypropanenitrile anodic oxidn electrochem
IT Oxidation, electrochemical
(of cyanoethanol to cyanoacetic acid)
IT **109-78-4**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(anodic oxidn. of)
IT 74-90-8P, preparation 6162-76-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in anodic oxidn. of cyanoethanol)
IT **372-09-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by anodic oxidn. of cyanoethanol)
IT **109-78-4**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(anodic oxidn. of)
RN 109-78-4 HCAPLUS
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



IT **372-09-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by anodic oxidn. of cyanoethanol)
RN 372-09-8 HCAPLUS
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)